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NON-EQUILIBRIUM RADIATION FOR THE HULL CODE

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AIR FORCE WEAPONS LABORATORY
Air Force Systems Command
Kirtland Air Force Base, NM 87117

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A treatment of flux-limited radiation diffusion is incorporated into the HULL code. The differential equations involved in the non-equilibrium radiation diffusion model are discussed, as well as the flux limiters. The difference equations used are also derived. The code has been exercised on several test problems and results from two of these test problems are reported.

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PREFACE

We would like to thank Dr. Clifford Rhoades for helpful discussions and assistance with the programming. Computer time was made available from Laboratory Director's Funds.

SECTION I

INTRODUCTION

HULL is a computer code that solves, within an Eulerian mesh, the hydrodynamic equations of continuity, momentum, and energy with a finite difference scheme (ref. 1). The code has an equilibrium radiation diffusion treatment. However, the assumption of equilibrium diffusion severely limits the types of problems that can be addressed. Moreover, the manner in which the equilibrium diffusion is implemented requires an unacceptably small timestep. For these reasons we have incorporated a treatment of non-equilibrium radiation diffusion that includes a flux-limiter for optically thin regions.

Non-equilibrium diffusion relaxes the assumption that the material and radiation must have the same temperature. However, we have not included a multi-frequency treatment, so we are still forced to assume the radiation field has a black body distribution, although the black body temperature is not required to be equal to the material temperature. The flux-limiters have been added to extend the diffusion theory to optically thin regions. The diffusion coefficient is modified so that the flux goes over to the free-streaming results when the mean-free-path becomes long.

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1. HULL Hydrodynamic Computer Code, AFWL TR 76-183, Air Force Weapons Laboratory, Kirtland AFB, NM 87117, (1976).

SECTION II

THE DIFFUSION EQUATION IN CYLINDRICAL COORDINATES

We write the diffusion equation in cylindrical coordinates as

$$\frac{\partial E}{\partial t} + \frac{1}{R}\frac{\partial}{\partial R}(RF_R) + \frac{\partial}{\partial Z}F_Z$$

$$= \rho\kappa_a c(aT^4 - E)$$

and the associated change in the material energy density as

$$\frac{\partial E_m}{\partial t} = -\rho\kappa_a c(aT^4 - E)$$

Here E is the radiation energy density, ρ is the material density, κ_a is the absorption opacity, c is light velocity, a is the radiation constant, T is the material temperature, E_m is the material energy density, and F_R and F_Z are the radiation fluxes in the R and Z directions, respectively. This equation incorporates the non-equilibrium diffusion approximation; the radiation energy density is not assumed to be aT^4, the black body energy density. We note that no material radiation energy exchange due to Compton scattering is included. While we do not incorporate the Compton energy exchange, Compton scattering is included in the diffusion coefficients and hence in the computation of the radiation fluxes.

The material-radiation energy exchange is done with the operator splitting method as discussed, for example, by Richtmyer (ref.2). Operator splitting is also used to solve the diffusion equation; we do the R diffusion separately from the Z diffusion.

F_R and F_Z are taken to be

$$F_R = -f_R\frac{c\lambda}{3}\frac{\partial E}{\partial R}$$

2. Richtmyer, R., and Morton, K., Difference Methods for Initial-Value Problems, Interscience Publishers, New York, 1967.

and

$$F_Z = - f_Z \frac{c\lambda}{3} \frac{\partial E}{\partial Z}$$

where λ is the total mean free path (absorption and scattering), and f_R are f_Z are the "flux-limiters" in the R and Z directions, respectively. f_R and f_Z are computed as

$$f_R = \frac{1}{1 + \frac{1}{3} \lambda \left| \frac{\partial \ln E}{\partial R} \right| \left(1 + 3 \exp\left\{- \frac{1}{2} \lambda \left| \frac{\partial \ln E}{\partial R} \right| \right\}\right)}$$

and

$$f_Z = \frac{1}{1 + \frac{1}{3} \lambda \left| \frac{\partial \ln E}{\partial Z} \right| \left(1 + 3 \exp\left\{- \frac{1}{2} \lambda \left| \frac{\partial \ln E}{\partial Z} \right| \right\}\right)}$$

We see that our expressions for F_R and F_Z are the standard diffusion fluxes except for the flux limiters. For small λ (when diffusion should apply), the flux limiters are near unity, and we have ordinary diffusion theory. When λ becomes sufficiently large (which depends on the scale of the problem) so that the diffusion approximation breaks down, the flux limiters reduce the diffusion coefficients so that the radiation flux cannot exceed the product of light velocity and the energy density, which is the maximum physically allowable flux. To see this limiter behavior, consider F_R with λ large. We neglect the exponential term since it has a negative argument of large absolute value. Then we have

$$F_R = - \frac{c\lambda}{3} \left(\frac{1}{1 + \frac{1}{3} \lambda \left| \frac{\partial \ln E}{\partial R} \right|} \right) \frac{\partial E}{\partial R}$$

or

$$F_R = - \frac{c\lambda}{3 + \lambda \frac{1}{E} \left| \frac{\partial E}{\partial R} \right|} \frac{\partial E}{\partial R}$$

Assuming λ is sufficiently large so that we may neglect the 3 in the denominator, we have

$$F_R = - \frac{\partial E/\partial R}{|\partial E/\partial R|} cE$$

That is, $|F_R| = cE$, with the direction of flow determined by the direction of the gradient in E.

Our discussion has been slightly misleading in that we have concentrated on the value of λ. Of more importance is the size of λ compared with ℓ_E where

$$\ell_E = \frac{1}{\left|\frac{\partial \ \ell n \ E}{\partial R}\right|} = \frac{E}{\left|\frac{\partial E}{\partial R}\right|}$$

ℓ_E is a radiation scale length (or scale height). If $\lambda >> \ell_E$, then the flux limiters become operational. However, if $\ell_E >> \lambda$, $f_R \approx f_Z \approx 1$, and we have normal diffusion.

A more complete description of flux limited diffusion theory is given by Winslow (refs. 3 and 4). As indicated by Winslow, much of the flux limiter development has been done by LeBlanc and Wilson of the Lawrence Livermore Laboratory.

---

3. Winslow, A.M., Improved Flux Limiter for Asymptotic Neutron Diffusion Calculations, UCIR-378, Lawrence Livermore Laboratory, Livermore, CA, April 1969.
4. Winslow, A.M., "Extensions of Asymptotic Neutron Diffusion Theory," Nuclear Science and Engineering, 32, pp 101-110, 1968.

SECTION III

DIFFERENCE EQUATIONS

We adopt operator splitting methods (e.g., ref. 2) to separate our diffusion equation into a radial component and an axial component, each of which is separately solved numerically. Half of the radiation-material coupling is done with each radiation sweep. That is, we assume

$$\frac{\partial E}{\partial t} = \frac{\partial E}{\partial t}\Big|_R + \frac{\partial E}{\partial t}\Big|_Z$$

and

$$\frac{\partial E_m}{\partial t} = \frac{\partial E_m}{\partial t}\Big|_R + \frac{\partial E_m}{\partial t}\Big|_Z$$

where

$$\frac{\partial E}{\partial t}\Big|_R = -\frac{1}{R}\frac{\partial}{\partial R}(RF_R) + \frac{1}{2}\rho\kappa_a c(aT^4 - E)$$

$$\frac{\partial E}{\partial t}\Big|_Z = -\frac{\partial}{\partial Z}F_Z + \frac{1}{2}\rho\kappa_a c(aT^4 - E)$$

and

$$\frac{\partial E_m}{\partial t}\Big|_R = \frac{\partial E_m}{\partial t}\Big|_Z = -\frac{1}{2}\rho\kappa_a c(aT^4 - E)$$

We first derive the radial difference equation in detail. The fully implicit difference equations are

$$E - E^\circ = \frac{\Delta t}{R\Delta R}\left(\frac{Rc\lambda}{3}\Big|_{+1/2}\frac{E_+ - E}{R_+ - R} - \frac{Rc\lambda}{3}\Big|_{-1/2}\frac{E - E_-}{R - R_-}\right) + \frac{\rho\kappa_a c\Delta t}{2}(aT^4 - E)$$

and

$$E_m - E_m^\circ = -\frac{\rho\kappa_a c\Delta t}{2}(aT^4 - E)$$

where the $E°$, $E_m°$, and T_o denote the quantities at the beginning of the current time step. Unless otherwise indicated, the quantities are cell centered. Here + (-) refers to the adjacent cell center at larger (smaller) radius. We use +1/2 (-1/2) to indicate the boundary between the current cell and the + (-) cell. Note that ΔR(no subscript) is computed as $\Delta R = R_{+1/2} - R_{-1/2}$. These equations, coupled with the equation of state, completely determine E, E_m, and T. In order to calculate these quantities, we first make the approximation

$$E_m - E_m^\circ = \rho C_v (T - T_o)$$

where C_v is the material specific heat. We are then faced with solving a 4th order system in T. We choose to solve this system by linearizing the 4th order term.

The linearization is taken to be

$$T^4 = T_o^4 + 4T_o^3 (T - T_o)$$

$$= 4T_o^3 T - 3T_o^4$$

Then

$$E - E^\circ = - \frac{\Delta t}{R\Delta R} \left\{ \frac{Rc\lambda}{3\Delta R} \bigg|_{+1/2} (E_+ - E) - \frac{Rc\lambda}{3\Delta R} \bigg|_{-1/2} (E - E_-) \right\} + \frac{\rho\kappa_a c\Delta t}{2} \left\{ 4aT_o^3 T - 3aT_o^4 - E \right\}$$

and

$$\rho C_v (T - T_o) = - \frac{\rho\kappa_a c\Delta t}{2} \left\{ 4aT_o^3 T - 3aT_o^4 - E \right\}$$

Collecting terms, we have

$$T\left\{1 + \frac{\rho\kappa_a c\Delta t}{2\rho C_v} 4aT_o^3\right\} = T_o + \frac{\rho\kappa_a c\Delta t}{2\rho C_v}\left\{3aT_o^4 + E\right\}$$

Now define δ as

$$\delta \equiv \frac{\rho\kappa_a c\Delta t}{2\rho C_v}$$

Then

$$T(1 + \delta 4aT_o^3) = T_o + \delta(3aT_o^4 + E)$$

or solving for E,

$$E = \frac{T(1 + \delta 4aT_o^3) - T_o(1 + \delta 3aT_o^3)}{\delta}$$

$$= \frac{(T - T_o)(1 + \delta 4aT_o^3) + \delta aT_o^4}{\delta}$$

$$= (T - T_o)\left[\frac{1 + \delta 4aT_o^3}{\delta}\right] + aT_o^4$$

so

$$T - T_o = \frac{\delta}{1 + \delta 4aT_o^3}\left[E - aT_o^4\right]$$

Concentrating on the material interaction terms, we have

$$E - E^\circ = \frac{\rho\kappa_a c\Delta t}{2}\left[4aT_o^3(T - T_o) + aT_o^4 - E\right]$$

$$= \frac{\rho\kappa_a c\Delta t}{2}\left[\frac{4aT_o^3\delta}{1 + \delta 4aT_o^3}(E - aT_o^4) - (E - aT_o^4)\right]$$

$$= (aT_o^4 - E)\,\frac{\rho\kappa_a c\Delta t}{2}\,\frac{1}{1 + 4aT_o^3\delta}$$

Then

$$E\left(1 + \frac{\rho\kappa_a c\Delta t}{2}\,\frac{1}{1 + 4aT_o^3\delta}\right) = E^\circ + \frac{\rho\kappa_a c\ t}{2}\,\frac{aT_o^4}{1 + 4aT_o^3\delta}$$

Adding the transport terms we have

$$E\left(1 + \frac{\Delta t}{R\Delta R}\cdot\frac{Rc\lambda}{3\Delta R}\bigg|_{+1/2} + \frac{\Delta t}{R\Delta R}\cdot\frac{Rc\lambda}{3\Delta R}\bigg|_{-1/2} + \frac{\rho\kappa_a c\Delta t}{2}\,\frac{1}{1 + 4aT_o^3\delta}\right)$$

$$= E_+\frac{\Delta t}{R\Delta R}\cdot\frac{Rc\lambda}{3\Delta R}\bigg|_{+1/2} + E_-\frac{\Delta t}{R\Delta R}\cdot\frac{Rc\lambda}{3\Delta R}\bigg|_{-1/2}$$

$$+ E^\circ + \frac{\rho\kappa_a c\Delta t}{2}\,\frac{aT_o^4}{1 + 4aT_o^3\delta}$$

Finally,

$$T = T_o + \frac{\delta}{1 + \delta'}(E - aT_o^4)$$

where

$$\delta' = \delta 4aT_o^3$$

Then

$$E_m = E_m^\circ + \rho C_v\,\frac{\delta}{1 + \delta'}(E - aT_o^4)$$

SECTION IV

TEST PROBLEMS

We have run two classes of test problems. First, we have calculated the propagation of plane waves parallel to the z axis and compared the results with an established one-dimensional code. Second, we have placed a spherical source in the center of the two-dimensional mesh and followed the radiation front to test the symmetry characteristics of the difference equations.

As an example of the plane wave problems, we present results from a calculation with 40 cells in the z direction. The source region consisted of the first five rows with energies of 2×10^{14} ergs/gm while the remainder of the mesh was filled with an ambient energy of 10^{12} ergs/gm. Reflective boundary conditions were used on all boundaries. Cells were 250 cm square, and the mean free path was 7500 cm (30 cells). Circles with dots in figure 1 indicate the flux for each of the first 28 zones after 20 cycles. For our comparison we have chosen a one-dimensional code that employs a similar radiation flux-limited diffusion scheme (ref. 5). Identical initial conditions were used in this code, and the results are shown as x's in figure 1. The agreement is excellent - the slight differences in the flux for the outer cells is the result of using a different procedure to calculate an average opacity for the outer boundary in the two codes.

The second case used a mesh of 100 x 100 cells with cell dimensions equal to 50 cm. Our spherical source with an energy density of 2×10^{14} ergs/gm had a radius of 25 zones. The mean free path was fixed at 1000 cm (20 cells). Figures 2 and 3 show the initial conditions of this calculation for material energy density and radiation energy density. Figures 4, 5, 6, and 7 illustrate the expanding source.

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5. Alme, M.L. and Wilson, J.R., "Numerical Study of Accretion onto a Neutron Star," Astrophysical Journal, 186, p 1015, 1973.

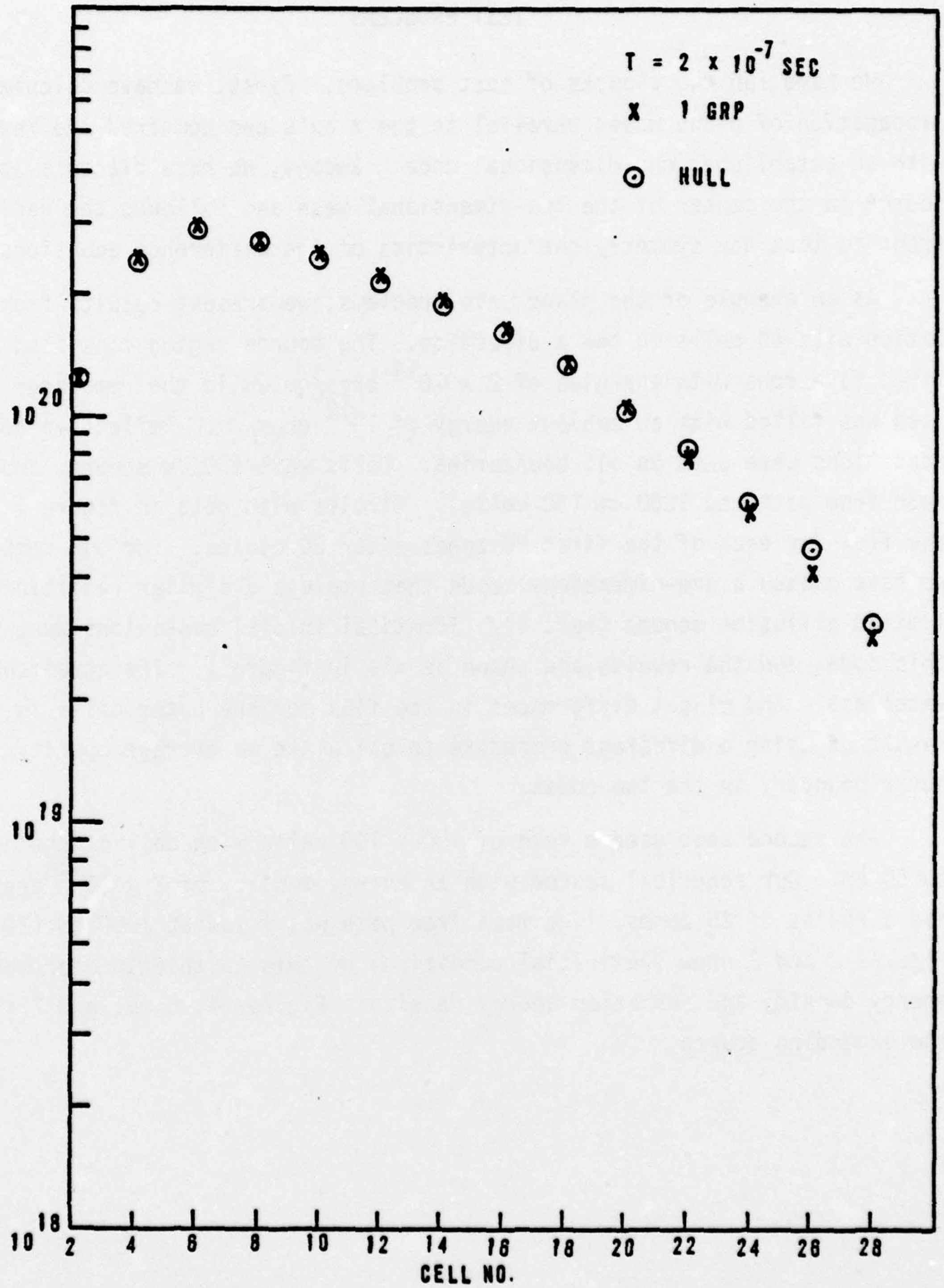

Figure 1. Comparison of HULL Non-Equilibrium to 1-D Code

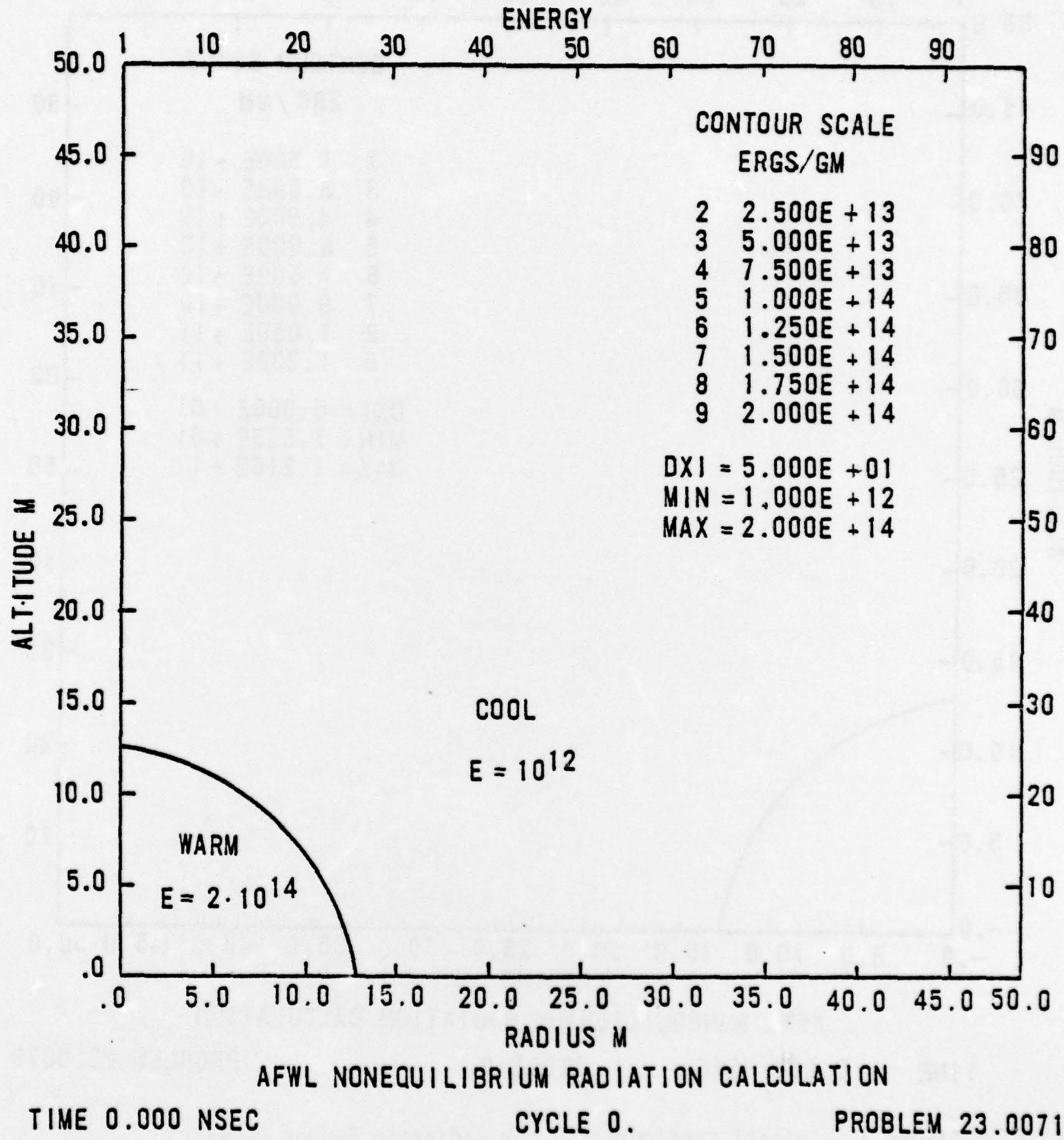

Figure 2. Initial Configuration for Material Energy Density

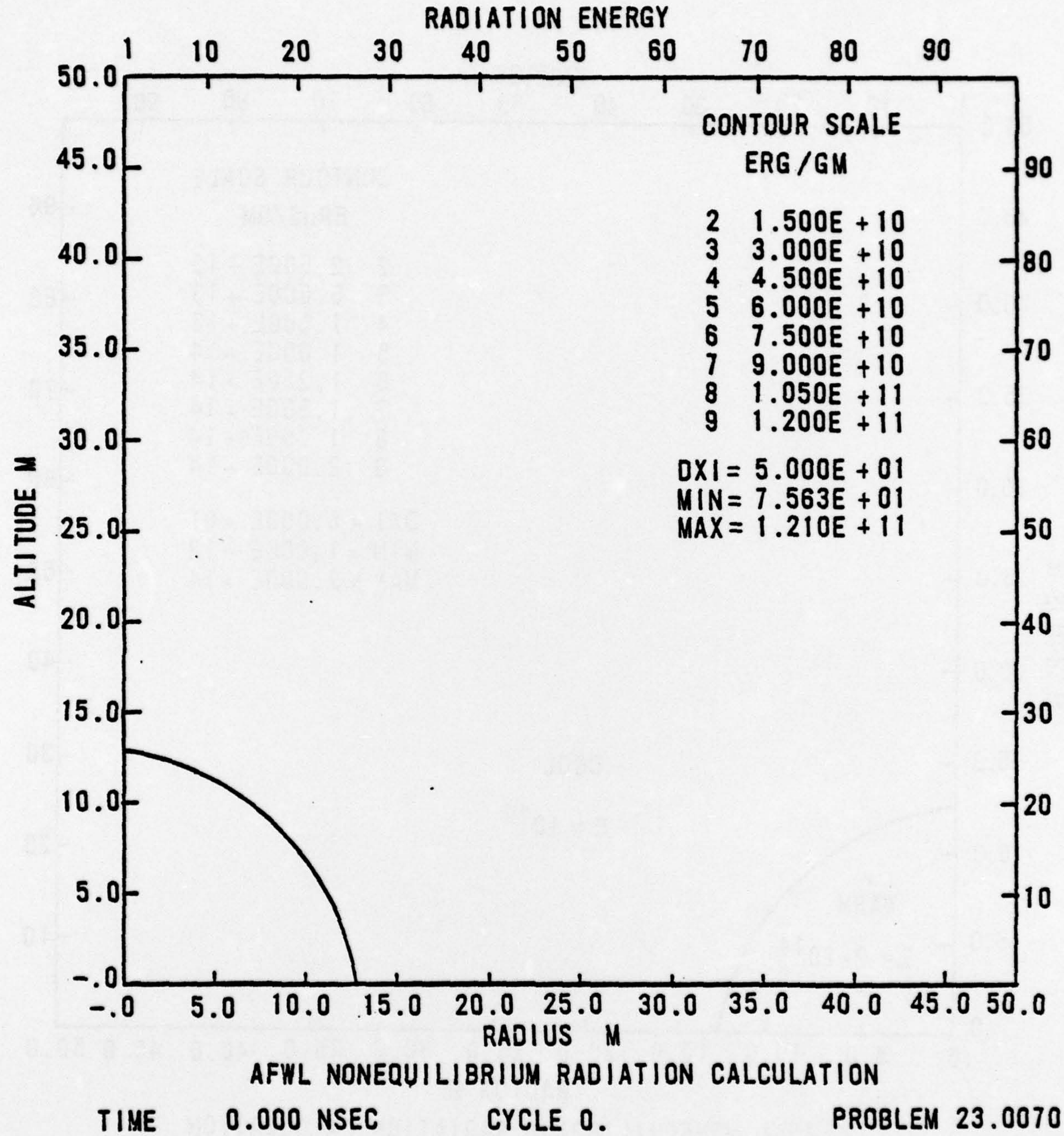

Figure 3. Initial Configuration for Radiation Energy Density

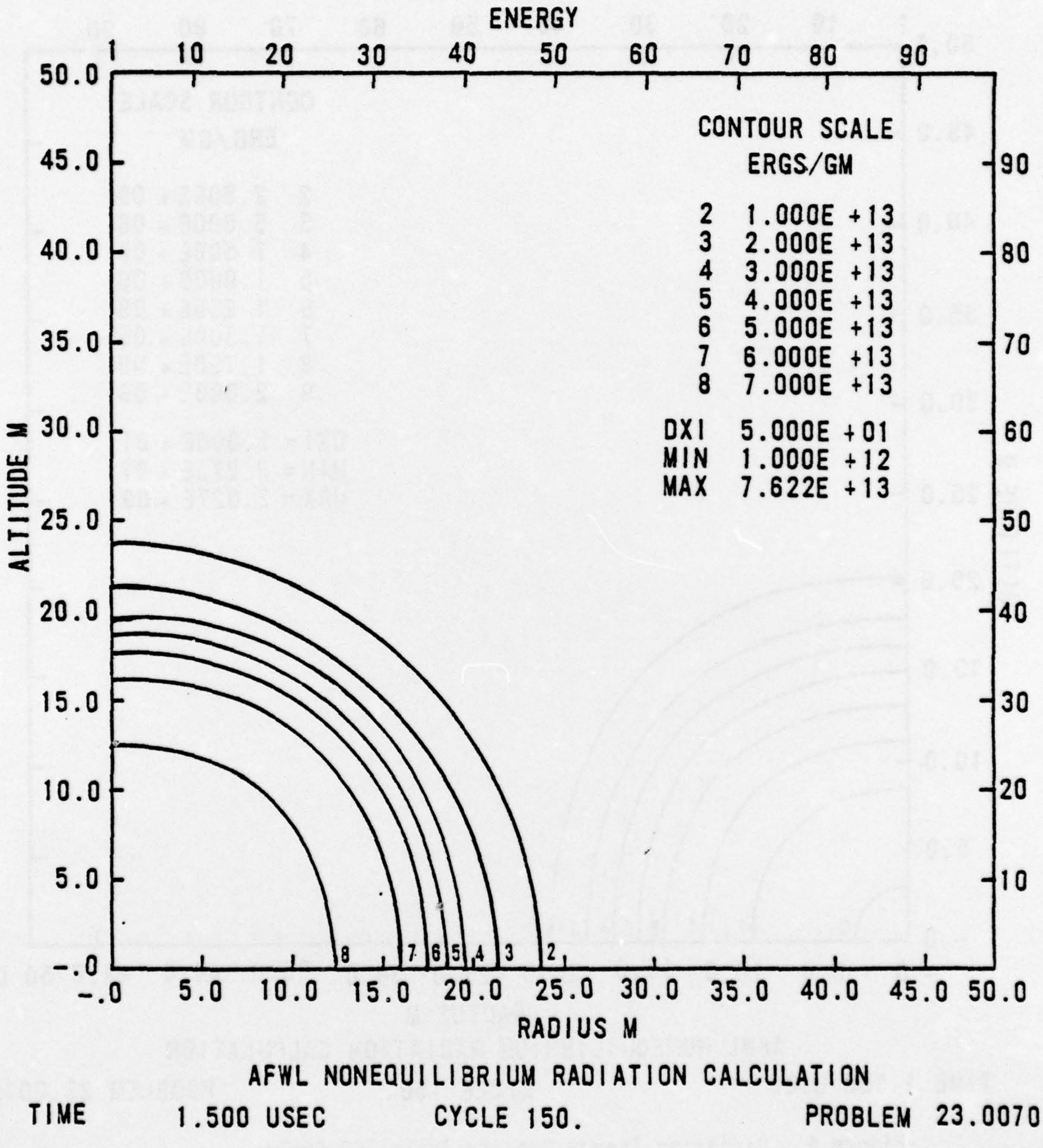

Figure 4 Material Energy After 150 Cycles

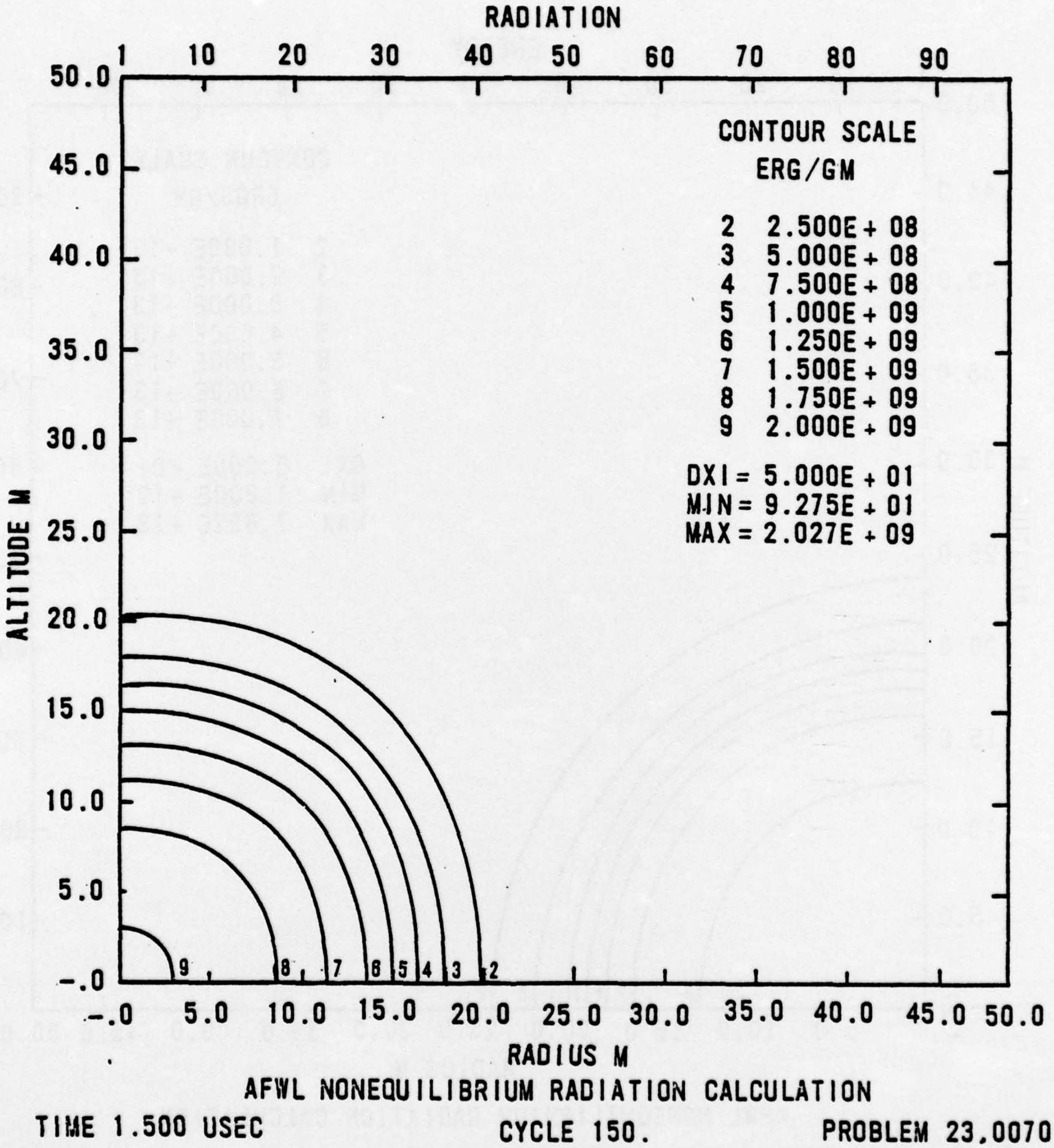

Figure 5. Radiation Energy Density After 150 Cycles

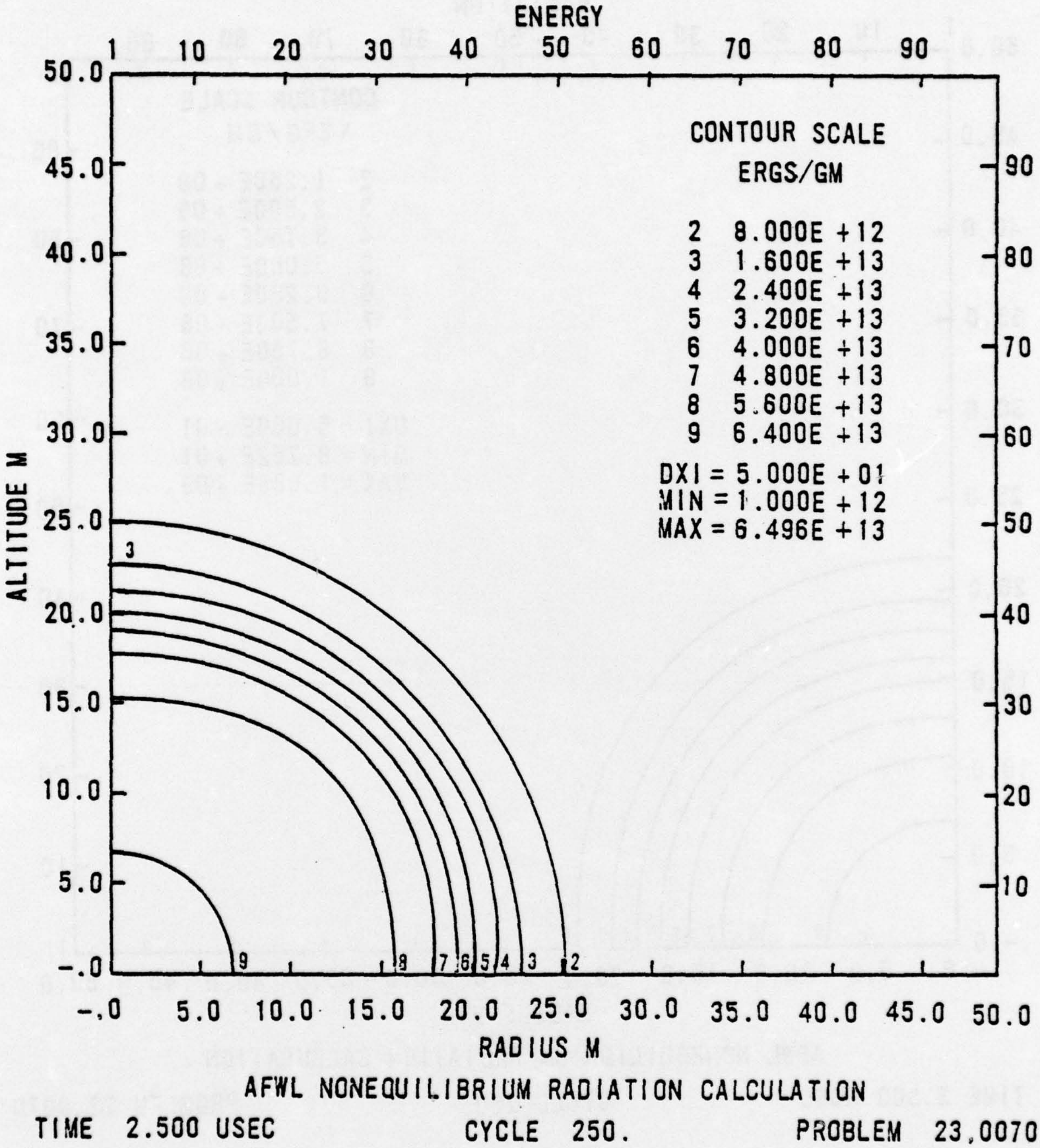

Figure 6. Material Energy Density After 250 Cycles

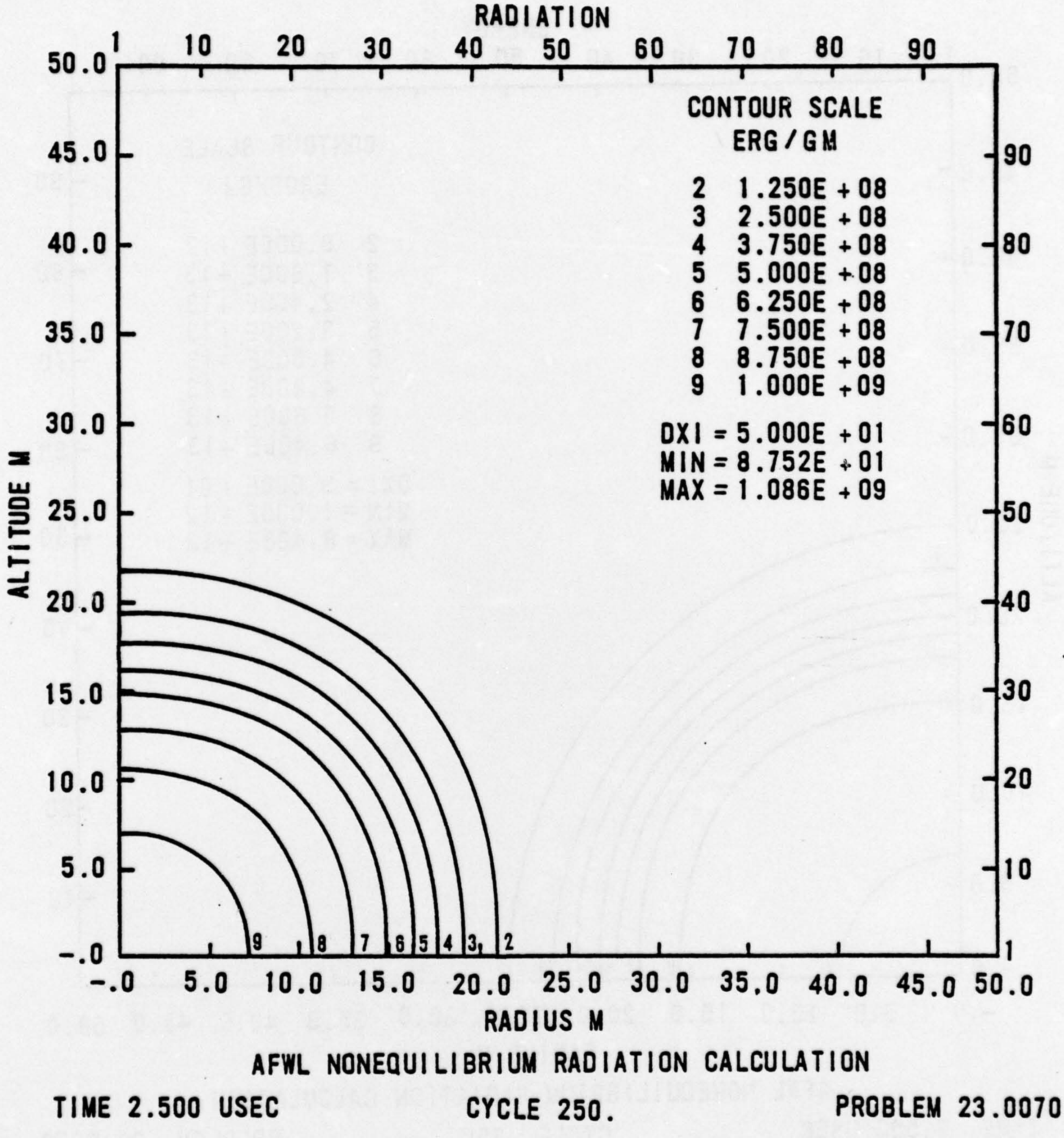

Figure 7. Radiation Energy Density After 250 Cycles

REFERENCES

1. HULL Hydrodynamic Computer Code, AFWL TR 76-183, Air Force Weapons Laboratory, 1976.
2. Richtmyer, R., and Morton, K., Difference Methods for Initial-Value Problems, Interscience Publishers, New York, 1967.
3. Winslow, A.M., Improved Flux Limiter for Asymptotic Neutron Diffusion Calculations, UCIR-378, Lawrence Livermore Laboratory, Livermore, CA April 1969.
4. Winslow, A.M., "Extensions of Asymptotic Neutron Diffusion Theory," Nuclear Science and Engineering, 32, pp 101-110, 1968.
5. Alme, M.L. and Wilson, J.R., "Numerical Study of Accretion onto a Neutron Star," Astrophysical Journal, 1868, p 1015, 1973.